Current Status of the Development and Application of Mesoscale and Global WRF/Chem at NCSU

Yang Zhang, Xin-Yu Wen, Xiao-Ming Hu, Ying Pan, Joshua Hemperly, and Nicholas Meskhidze North Carolina State University

DOE ASP FY 2008 Science Team Meeting, 25–27 February, 2008, Annapolis, MD



Weather Research and Forecast/Chemistry Model (WRF/Chem) at NCSU: Overview

Key Collaborators

- G. Grell, S. Peckham, and S. McKeen, NOAA-ESRL
- J. Fast, W. Gustafson Jr., R. Easter, R. Zaveri, and S. Ghan, PNNL
- K. Schere, T. Otte, J. Pleim, G. Sarwar, J. Herwehe, and S.T. Rao, U.S. EPA/NOAA-ASMD, C. Jang, EPA/OAQPS
- W. Skamarock, NCAR-MMMD; L. Emmons and F. Vitt, NCAR-ACD

History and Milestones

- Jan., 2004: Code installed and operational at NCSU
- 2004: Incorporation of MADRID into WRF/Chem
- 2005: Testing, application, evaluation over TeXAQS2000 (WRF 2005, AGU 2005)
- 2006: Incorporation of CB05 and evaluation (AMS, 2006, WRF 2006, CMAS 2006)
- 2007-present:
 - Application at 36-km over CONUS (WRF 2007, CMAS 2007, AMS 2008)
 - Testing of WRF/Chem-MADRID at 24-km over New England (CMAS 2007)
 - Implementation of CB05-KPP in WRF/Chem-MADRID (AMS 2008)
 - Development and Testing of Global WRF/Chem (AMS 2008)

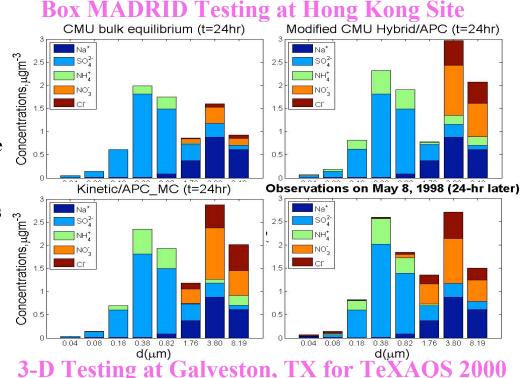
Gas and Aerosol Treatments in WRF/Chem

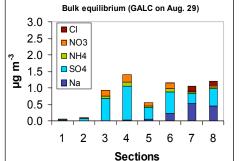
	MADE/SORGAM	MOSAIC	MADRID
Gas chemistry	RADM2/RACM	CBM-Z	CBM-Z/CB05
Size structure	Modal (3 modes)	Sectional (8 bins)	Sectional (8 bins)
Inorganic species		plus Na ⁺ , Cl ⁻	plus Na ⁺ , Cl ⁻
Equilibrium	MARS-A	MESA-MTEM	ISORROPIA
Coagulation	Modal	Sectional	Sectional
Nucleation	Binary	Binary	Binary
Condensation	Modal	Sectional	Sectional
Gas/Particle	Full equilibrium	Dynamic with	1. Full equilibrium
Mass transfer	•	ASTEEM	2. Dynamic
			3. Hybrid
SOA formation	Reversible absorption (8 classes VOCs)	Same as MADE/SORGAM	MADRID 1: Reversible absorp. (39 VOCs) MADRID 2: Reversible absorp. and dissolution (42 VOCs)
Dry deposition	Resistance transfer with a simple parameterization for $\boldsymbol{V}_{\boldsymbol{d}}$	Resistance transfer	Resistance transfer

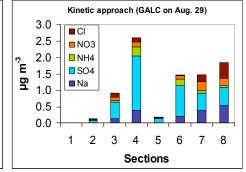
Development Highlights: Incorporation of MADRID into WRF/Chem

Gas/Particle Mass Transfer

- Bulk equilibrium
- Hybrid
- Kinetic
- Objectives
 - Identify limitations/advantages
 - Develop a computationally-efficient module
- Approaches
 - Box model development
 - Evaluation using size-resolved observations
 - 3-D model testing
- 3-D Testbeds
 - TeXAQS 2000 (12-km)
 - New England 2004 (27-km)
 - **CONUS 2001 (36-km)**
- Major Findings
 - Bulk equilibrium approach fails to predict semi-volatile species in areas with active coarse PM, where kinetic approach is needed
 - Kinetic and hybrid approaches take 1.8-3.6 and 1.05 times more CPU than bulk equilibrium
 - Gases and size-resolved PM measurements are needed (e.g., ASP)



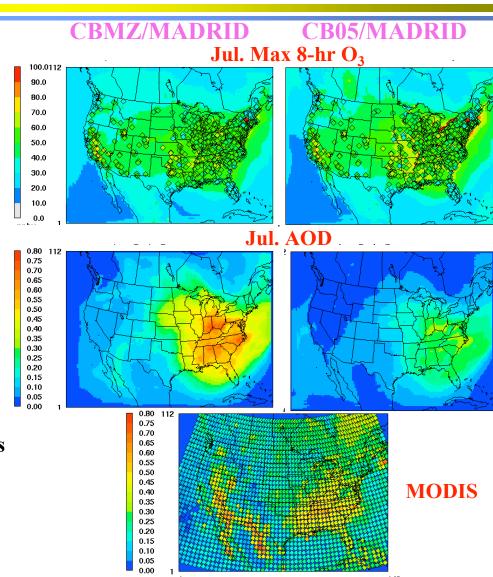




Development Highlights: Implementation of CB05_KPP in WRF/Chem-MADRID

Gas-Aerosol Coupling

- CBMZ-MADRID
- CB05-MADRID
- SAPRC99-MADRID
- Objectives
 - Examine sensitivity of aerosol predictions to gas chemistry
 - Improve SOA treatment
- Approaches
 - Implementation of CB05_KPP
 - Intercomparison with CBMZ/MADRID
 - Evaluation using observations
- 3-D Testbeds
 - Jul. 2001 CONUS (36-km)
 - Jul./Jan. 2005 Asia (36-km)
- Major Findings
 - WRF/Chem shows reasonably-good skills for surface O₃/PM_{2.5}, column NO₂ and CO, but relatively poor performance for TOR in Jul. and AOD in Jan.
 - CB05 gives higher O₃, CO, and HCHO; lower NO_x, HNO₃, PM_{2.5}, and its inorganic components



Development Highlights:

Global-through-Urban WRF/Chem (GU_WRF/Chem)

Key Development

- Extension of CB05
- Addition of Hg chemistry
- Improvement of aerosol treatments
- Addition of plume-in-grid treatments

Objectives

- Develop a unified model framework for multiscale modeling
- Apply it to replicate and examine climatechemistry-aerosol-cloud feedbacks

Approaches

- Couple chemistry with global WRF
- Expand chemistry to represent globe
- Evaluation using observations

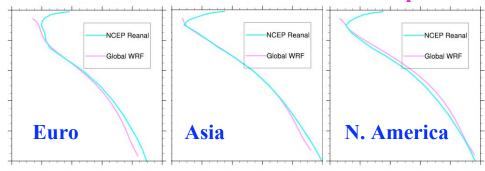
3-D Testbeds

- Jan., Jul., Aug. 2001 (1.125° × 1.125°)
- Jan./Jul. 2001 $(4^{\circ} \times 5^{\circ})$

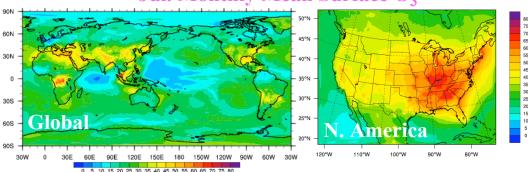
Major Findings

- G-WRF/Chem demonstrates some skills
- Goddard shortwave scheme outperforms
 Dudhia scheme
- Reinitialization is needed
- Upper BCs need to be improved

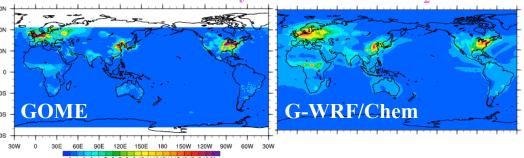
Vertical T Profile over Northern Hemisphere



Jul. Monthly Mean Surface O₃



Jan. Monthly Mean Column NO2

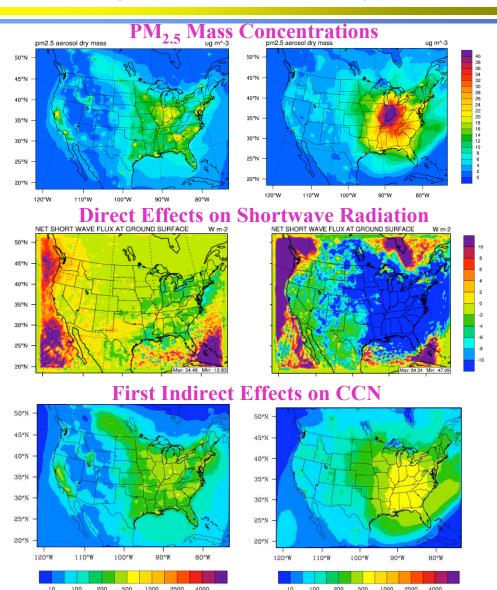


Application Highlights: Aerosol-Radiation-Cloud Feedbacks with WRF/Chem-MOSAIC

Jan. Jul.

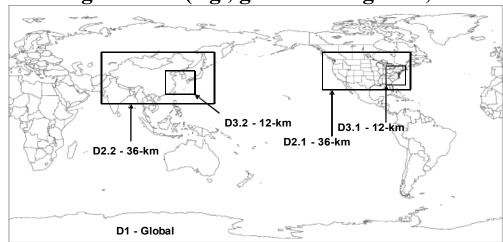
Objectives

- Test model configurations
- Examine aerosol-radiation-cloud feedbacks
- Assess impact of climate change on AQ
- Approaches
 - Met; Met+Gas; Met+Gas+PM+Cloud
 - Seasonal contrast (Jan. vs. Jul.)
 - Evaluation using observations
- 3-D Applications
 - TeXAQS 2000 (12-km)
 - Jan./Jul. 2001 CONUS (36-km)
 - Jan./Jul. 2005 Asia (36-km)
- Preliminary Findings
 - PM can decrease shortwave radiation,
 T, and PBLH; increase CCN, and affect
 JNO₂, SH, WSP, and precip. in
 different ways
 - Overall stronger feedbacks in Jul. than Jan., and over EUS than WUS
 - Data are needed to verify simulated feedbacks (e.g., ASP)



Planned Model Development and Applications

- Meso- and Global-WRF/Chem
 - Emissions: global, online emission module for dust, plume-in-grid
 - Gas-phase and PM chemistry: CB05, SAPRC99, stratospheric, chlorine, Hg
 - Aerosol treatments: nucleation, coagulation, SOA, aerosol activation
- Applications (DOE CCPP/ASP)
 - Current-year: CAM4/MIRAGE (2001-2005) and GU-WRF/Chem (2001)
 - Future-year: CAM4/MIRAGE (2050-2054) and GU-WRF/Chem (2050)
 - Sensitivity:
 - model inputs (e.g., BVOC emissions from land/ocean)
 - model formulations (e.g., SOA, new PM formation, aerosol-cloud inter.)
 - model configurations (e.g., global vs. regional, fine vs. coarse resolutions)



Acknowledgments and Disclaimer

- Project Sponsors: NSF, NOAA, EPA, and DOE
- Jerome Fast, William Gustafson Jr., Rahul Zaveru, Richard Easter, and Steven Ghan, PNNL, for providing PNNL's WRF/Chem code.
- Georg Grell, Steve Peckham, and Stuart McKeen, NOAA/ESRL, for helpful discussions on WRF/Chem options.
- S.T. Rao, Ken Schere, George Pouliot, and Golam Sarwar, Jonathan Pleim, Tanya Otte, and Robert Gilliam, Alice Gilliland and Steve Howard, and Shaocai Yu, U.S. NOAA/AMD, for providing WRF and CMAQ inputs for regional WRF/Chem simulations; Fortran code for extracting data from observational databases and CMAQ; and Fortran code for statistical calculation.
- Mark Richardson, Caltech, and William Skamarock, NCAR/MMMD, for sharing global WRF.
- Andreas Richter, the University of Bremen, Germany, for providing GOME NO₂ data; Hilary E. Snell, AER Inc., for processing GOME NO₂; Jack Fishman and John K. Creilson, NASA Langley Research Center, for providing TOR data.
- John Seinfeld and Daven Henze, Caltech, for providing isoprene SOA yield parameters based on their smog chamber data for model incorporation.
- Chak Chan, HKUST, for providing size-resolved PM measurements.

This work constitutes a contribution to the NOAA Air Quality Program.